Phase diagram of the metal-insulator transition in 2D electronic systems

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We investigated the interdependence of the effects of disorder and carrier correlations on the metal-insulator transition in two-dimensional electronic systems. We present a quantitative metal-insulator phase diagram. Depending on the carrier density we find two different types of metal-insulator transition – a continuous localization for $r_s \lesssim 8$ and a discontinuous transition at higher r_s. The critical level of disorder at the transition decreases with decreasing carrier density. At very low carrier densities we find that the system is always insulating. The value of the conductivity at the transition is consistent with recent experimental measurements. The self-consistent method which we have developed includes the effects of both disorder and correlations on the transition, using a density relaxation theory with the Coulomb correlations determined from numerical simulation data.

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A metal-insulator transition (MIT) has now been observed in a number of different 2D electronic systems over a wide range of carrier densities and levels of disorder. At the transition the carrier density parameter r_s, which measures the strength of the carrier correlations, covers values $7 \lesssim r_s \lesssim 35$. [1–3] The strength of disorder at the transition also covers a wide range, and depends on the value of the critical r_s. In Si/SiGe [3] the transition occurs at low carrier densities and high mobilities. For the transition in Si MOSFETs which occurs at higher densities, the mobilities are much smaller. A recent experimental phase diagram [4] provides a relation between the strength of the correlations and the disorder. It shows that the critical level of the disorder at the transition diminishes as the correlations grow stronger.

In spite of a great deal of experimental and theoretical work the nature of the conducting state remains unclear and controversial. Unlike conventional metals, its Coulomb interaction energy is typically an order of magnitude larger than its Fermi energy. Numerous proposals have been made about the causes of the stabilization of this conducting phase. These include strong Coulomb repulsions between the carriers [5,6], or an anomalous enhancement of the spin-orbit interaction due to the broken inversion symmetry of the confining potential well in Si MOSFETs [7]. References [8] proposed that the conducting phase is superconducting, with the pairing of the carriers being mediated by the dynamic correlation hole surrounding each carrier. Thakur and Neilson [9] demonstrated the existence of superconducting pairing due to strong Coulomb correlations in the presence of disorder. They found up to levels of disorder typical of high quality Si MOSFETs that the superconductivity persists.

The conducting phase is destroyed not only at low but also at high carrier densities. Kravchenko *et al* [1] originally observed the insulator-to-metal transition by increasing the carrier density. Recently it has been reported that if the carrier density is increased further there is an upper critical value where the conducting phase again becomes unstable and the system enters another insulating phase [4]. This insulating phase has the characteristics of a single-particle localized state, while the insulating phase at low densities is a coherent insulator with properties similar to a Wigner crystal or glass. The critical density for the second transition, typically around $r_s \lesssim 7$, is still not low enough for electron interactions to be neglected. In this paper we treat Coulomb interactions and disorder on an equal footing in order to investigate the transitions at both small and large r_s.

In the strong correlation limit and in the absence of disorder, electrons localize to form a Wigner solid with long range crystalline order. Here we consider interacting charge carriers in the presence of weak disorder which would destroy any long range order. We have previously proposed that strong Coulomb correlations in the presence of disorder can localize electrons into a coherent glassy insulator with liquid-like short-range order [5]. We studied the metal-insulator transition in terms of the ergodic to nonergodic transition of the charge density fluctuations. The possibility of localization into such a glassy state has also been discussed recently by Chakravarty *et al* [10].

We define the order parameter for the glass state as $f(q) = \lim_{t\to\infty} \Phi(q,t)$, where $\Phi(q,t) \equiv (N(q,t)|N(q,0))$ is the Kubo-relaxation function for the dynamical density variable $N(q,t)$. The normalized variable $N(q,t) = \rho(q,t)/\sqrt{\chi(q)}$, where $\rho(q,t)$ is the usual density fluctuation operator and $\chi(q)$ is the static susceptibility. When the order parameter is non-zero, spontaneous density fluctuations do not decay at infinite time and the system will be an insulator. Conversely if $f(q)$ is zero then our system is in a conducting phase. Since our order parameter would be zero for any conducting phase it gives no indication about the precise nature of the conducting phase.

Within the Mori-Zwanzig formalism [11] $\Phi(q,t)$ is calculated in terms of the memory function $M(q,t)$, which we evaluate using mode-coupling theory [12]. In the limit

$t \to \infty$ the relaxation function reduces to

$$f(q) = \frac{1}{1 + \Omega(q)/M(q)} \ , \tag{1}$$

where $\Omega(q) = q^2/(m^\star \chi(q))$ and $M(q) = \lim_{t\to\infty} M(q,t)$. $m^\star$ is the carrier effective mass. We express $M(q) = M_{cc}(q) + M_{ic}(q)$, where

$$M_{cc}(q) = \frac{1}{2m^* q^2} \sum_{q'} [V(q')(\boldsymbol{q}\cdot\boldsymbol{q}') + V(|\boldsymbol{q}-\boldsymbol{q}'|) \times (\boldsymbol{q}\cdot(\boldsymbol{q}-\boldsymbol{q}'))]^2 \chi(q')\chi(|\boldsymbol{q}-\boldsymbol{q}'|) f(q') f(|\boldsymbol{q}-\boldsymbol{q}'|)$$

$$M_{ic}(q) = \frac{1}{m^* q^2} \sum_{q'} \left[n_i \langle |U_{\rm imp}(q)|^2 \rangle + \langle |W_{\rm surf}(q)|^2 \rangle \right] \times (\boldsymbol{q}\cdot\boldsymbol{q}')^2 \chi(|\boldsymbol{q}-\boldsymbol{q}'|) f(|\boldsymbol{q}-\boldsymbol{q}'|). \tag{2}$$

The $M_{cc}(q)$ part of the memory function originates from the interactions between the carriers, and the $M_{ic}(q)$ from the carrier-disorder interactions. $V(q) = 2\pi e^2/\epsilon q$ is the Coulomb potential with dielectric constant ϵ. $U_{\rm imp}(q)$ is the carrier-impurity potential for randomly distributed monovalent Coulombic impurities of density n_i which are embedded in the carrier layer. $W_{\rm surf}(q)$ is the surface roughness scattering term. Details of the disorder potentials used are given in Ref. [5].

To evaluate the static susceptibility $\chi(q)$ with correlations, we use the generalized Random Phase Approximation expression,

$$\chi(q) = \chi_0(q)/\{1 + V(q)(1 - G(q))\chi_0(q)\}, \tag{3}$$

where $\chi_0(q)$ is the Lindhard function for non-interacting electrons. The local field factor $G(q)$ accounts for the correlations between the carriers. We evaluate $G(q)$ from ground state properties of the electron liquid [13] using the fluctuation-dissipation theorem [14].

The memory functions $M_{cc}(q)$ and $M_{ic}(q)$ mutually influence each other through $f(q)$. The nature of the localized state at the transition is largely determined by which of these memory functions is dominant. At low densities and small levels of disorder the interactions between the carriers dominate and $M_{cc}(q)$ is much larger than $M_{ic}(q)$. In this case the localization is primarily caused by many-body effects and the localized state is a coherent frozen insulator. At the transition the order parameter $f(q)$ jumps from zero to non-zero and the system undergoes a discontinuous transition. In contrast, at high densities and high levels of disorder, where the carrier-disorder scattering dominates, $M_{ic}(q)$ is much larger than $M_{cc}(q)$. The localization transition in this case is to a non-coherent state where the carriers localize independently. We find that this transition is continuous, with the order parameter $f(q)$ continuously increasing with disorder. Our model thus predicts the two distinct types of metal-insulator transition.

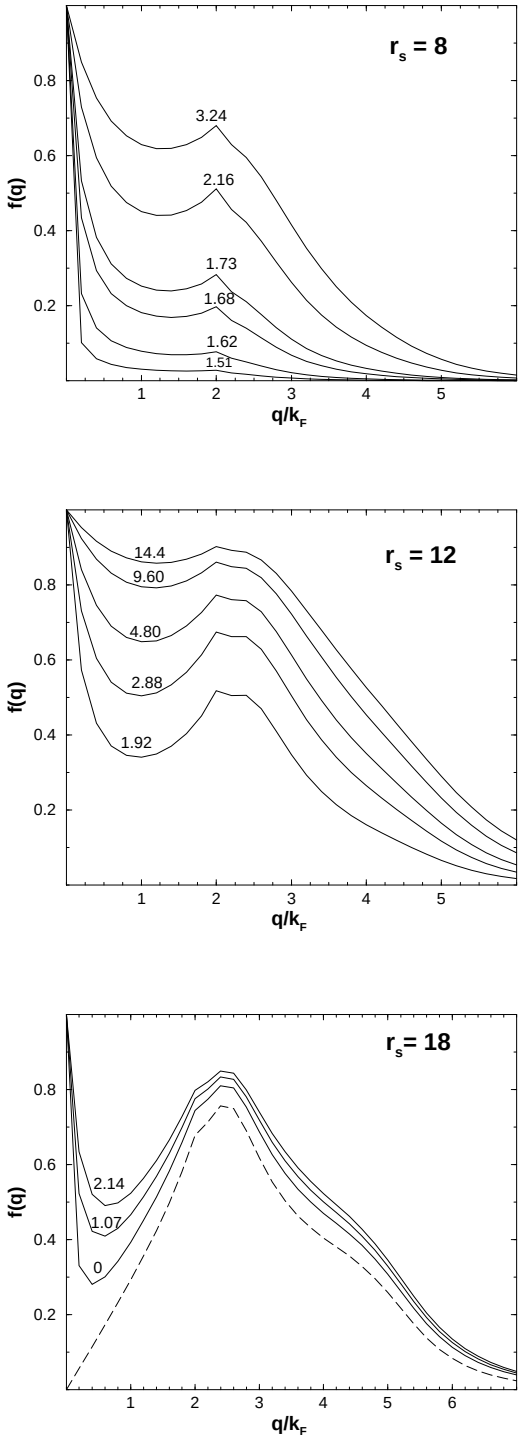

FIG. 1. Order parameter $f(q)$. Curve labels are impurity densities n_i. Surface roughness is included in all cases.
a. $r_s = 8$. n_i is in units of 10^{10}cm^{-2}.
b. $r_s = 12$. n_i is in units of 10^9cm^{-2}. $f(q)$ is zero for $n_i < 1.92 \times 10^9\text{cm}^{-2}$.
c. $r_s = 18$. n_i is in units of 10^8cm^{-2}. Dashed line is $n_i = 0$ with no surface roughness.

We solve Eqs. 1 and 2 self-consistently for the order parameter $f(q)$. We vary the strength of the disorder potential by varying the impurity density n_i while keeping the surface roughness at each r_s fixed.

In Fig. 1 we show the order parameter $f(q)$ for three values of $r_s = 8$, 12 and 18. The multiple curves for each fixed r_s correspond to increasing levels of disorder. At the highest carrier density, Fig. 1a, the localization is in general dominated by the $M_{ic}(q)$ part of the memory function. Here $f(q)$ increases continuously with impurity density, indicating continuous localization. These characteristic features that $f(q)$ evolves continuously with the disorder level and is non-zero for any disorder indicates a localized state where the particles localize independently. This is similar to Anderson-type localization. Since $f(q)$ is always non-zero there is no conducting phase when $r_s = 8$. The peak in $f(q)$ at $q = 2k_F$ is a result of the well–known cusp in the two-dimensional $\chi_0(q)$ and is of no importance here.

In contrast, in Fig. 1b for $r_s = 12$ the order parameter is zero for small non-zero levels of disorder. This indicates the existence of a conducting phase. If we increase the level of disorder, a critical value is passed at which $f(q)$ jumps discontinuously to non-zero values and at that point there is a metal-insulator transition [5]. The short-range coherent order of the insulator state is reflected by a peak in $f(q)$ at the reciprocal nearest neighbor distance, $q \approx 2.4k_F$. As we increase the disorder further, the $f(q)$ increases continuously. For very high levels of disorder, $n_i > 6 \times 10^9$ cm^{-2} , the overall shape of the $f(q)$ evolves towards a Gaussian indicating the development of a non-coherent insulator. We find in the range $8 \lesssim r_s \lesssim 18$ that the critical level of disorder required to localize the carriers decreases with increasing r_s and that the non-coherent state also occurs at decreasing n_i.

By $r_s = 18$ the system localizes without disorder and there is no conducting phase. This large r_s localization is driven purely by the correlations between the carriers. In Fig. 1c $f(q)$ is non-zero for $n_i = 0$ and no surface roughness scattering (dashed line). Without disorder the $f(q)$ goes to zero as q goes to zero. The solid lines show $f(q)$ with surface roughness scattering included.

The property that the critical level of disorder for the metal-insulator transition is dependent on the carrier density is associated with the changing strength of the correlations. The zero temperature phase diagram in Fig. 2 shows the relationship between the carrier density and the critical level of disorder at the transition. Disorder includes both the impurity density n_i and surface roughness. For $r_s \lesssim 8$ the system is insulating in the presence of any disorder, and the order parameter $f(q)$ is always non-zero. For $8 < r_s < 18$ the order parameter is zero for n_i less than a critical value and we have the conducting phase. At the right phase boundary the transition to the insulating phase is discontinuous and $f(q)$ jumps discontinuously to non-zero values as we cross it. The critical level of disorder for the transition decreases with decreasing density. Near the phase boundary where the disorder level is slightly larger than the critical value the system is in the coherent insulating state. For very large disorder the $f(q)$ has evolved into a Gaussian-like shape (see Fig. 1b) and the system becomes a non-coherent insulator. For $r_s \gtrsim 18$ the order parameter is non-zero without disorder and the conducting phase has disappeared. Our phase diagram has common features with the conceptual phase diagram discussed by Chakravarty *et al* [10].

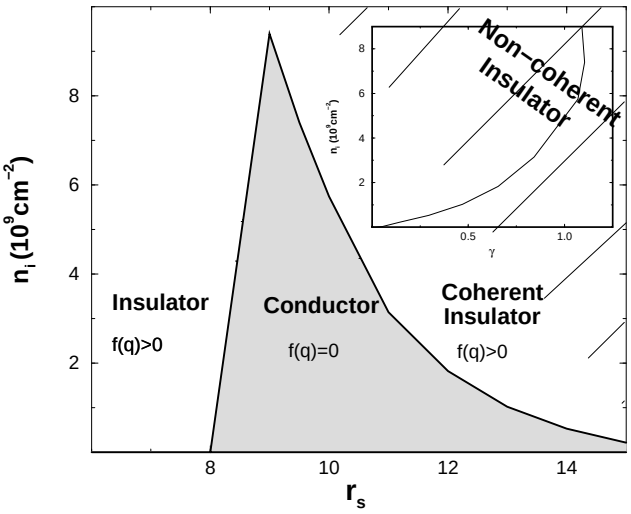

FIG. 2. Zero temperature phase diagram. Axes are impurity density n_i and carrier density parameter r_s. In the insulating phases the order parameter $f(q) > 0$. In the conducting phase $f(q) = 0$. The transition at higher densities is continuous. When $r_s > 9$ the $f(q)$ discontinuously jumps from zero to non-zero values at the transition. Inset shows the corresponding scattering rate $\gamma/(2E_F)$ at the transition as a function of n_i.

The inset in Fig. 2 shows the relation between n_i and the scattering rate γ off the disorder. Within the memory function formalism the non-linear equation for γ is given by [15]

$$\mathrm{i}\gamma = -\frac{1}{2m^\star n_c}\sum_q q^2\left[n_i\langle|U_{\rm imp}(q)|^2\rangle + \langle|W_{\rm surf}(q)|^2\rangle\right] \times\left(\frac{\chi(q)}{\chi^{(0)}(q)}\right)^2\frac{\phi_0(q,\mathrm{i}\gamma)}{1+\mathrm{i}\gamma\phi_0(q,\mathrm{i}\gamma)/\chi^{(0)}(q)}\ , \qquad (4)$$

where $\phi_0(q,\mathrm{i}\gamma) = (1/\mathrm{i}\gamma)\left[\chi^{(0)}(q,\mathrm{i}\gamma) - \chi^{(0)}(q)\right]$ is the relaxation spectrum for non-interacting carriers that scatter off the disorder. Thakur and Neilson [9] showed for the density range $5 \le r_s \le 10$ that the superconducting phase persists at least up to values of $\gamma/(2E_F) = 1$. They also showed that the effective potential becomes more strongly attractive as r_s increases. This suggests that our conducting phase in Fig. 2, which is only found for $\gamma/(2E_F) \lesssim 1$, is a superconductor.

Using the Drude model, γ can be related to the zero

temperature conductivity, $\sigma = (ne^2/m^\star)\gamma^{-1}$. In Fig. 3 we show σ at the transition as a function of r_s. In the range $9 < r_s < 14$, σ lies between $1 \lesssim \sigma/(e^2/h) \lesssim 3$. This is consistent with experimental values. At lower densities the σ calculated within the Drude model increases rapidly. This is associated with the decrease in the critical level of disorder at the transition. Since the Drude approximation is inapplicable for large r_s this increase in σ at low density should not necessarily be seen experimentally.

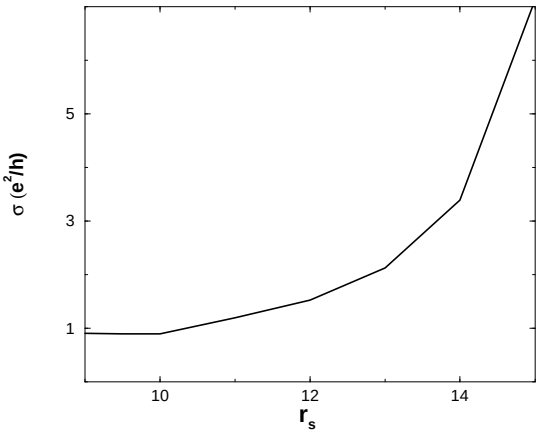

FIG. 3. Conductivity σ at the critical disorder for the transition as a function of r_s.

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